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EVALUATION OF LOCAL-SCALE MODELS FOR ACCIDENTAL RELEASES IN BUILT ENVIRONMENTS – RESULTS OF THE “MICHELSTADT EXERCISE” IN COST ACTION ES1006

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Abstract: Testing and evaluating available models by model inter-comparison, as well as by comparison against test data from qualified field and laboratory experiments is a main research task of COST Action ES1006. Assuming that a typical emergency response model has already been validated with regard to local-scale dispersion modelling, the existing model evaluation and validation strategies are extended towards task- and application-specific measures for accidental release scenarios, such as extreme value prediction and exposure assessment. In case of a continuous release, maximum concentrations, dosages and especially the area affected by values above a relevant threshold usually are the information expected from an emergency response model. In case of one or several puff releases, additional information may be of interest: When does the puff arrive at a certain point? How long is the duration of the puff passage at a point? What are the peak concentration values to be expected? The model evaluation focuses on the respective model output

Key words: *air pollution, model evaluation, accidental releases, emergency response.*

INTRODUCTION

The main tasks of the presented model evaluation case study for accidental continuous and puff releases in a typical European city “Michelstadt” (Fischer et al., 2010) are:

- Documenting the performance of modelling approaches,
- Quantifying the scatter of results when different models are applied,
- Quantifying the effect of uncertainties in input data.

Table 1 gives an overview of the source scenarios and respective numbers of receptor points measured in the wind tunnel for the COST ES1006 Michelstadt exercise. The results in the model validation dataset are provided as full scale values. For the conversion of the different variables from model scale to full scale, dimensionless numbers were used.

For the continuous release concentration data, beside the mean value and its uncertainty, the 5th, 95th and 99th percentiles and the maximum values are also provided for 15 s, 600 s, 1800 s and 3600 s averaging times. For the short-term (puff) releases, the distributions of puff parameters and their statistical values (such as median, mode, percentiles, skewness, etc.) are provided. To ensure sufficient statistical representativeness of the puff dispersion results, data from at least 200 consecutive releases was collected for each measurement location. For each individual release, the puff dispersion parameters are calculated and converted to full-scale conditions.

Table 1. Number of source locations and receptor points in COST ES1006 Michelstadt exercise

Experiments	**Number of source locations**	**number of receptor points**	
		Continuous	**puff releases**
non-blind	3	104	10
blind	4	248	31

The design of the experiment takes into account that hazardous releases may occur in very different locations in an urban area: in open squares, small or wide streets, perpendicular or parallel to the prevailing large-scale flow or even in court yards. As will be shown later, in general, the distribution of the plume from a release in a rather open part of the urban building structure (e.g. source 2 in Figure 1) should be well reproduced by most models while releases from a street perpendicular to the main flow or a court yard are affected by more complex flow structures in the vicinity of the source and thus, larger differences are to be expected between the measurements and the model simulations. On the other hand, the affected area also may comprise various building configurations. Therefore, receptor points also are situated in different surroundings as shown in Figure 1.

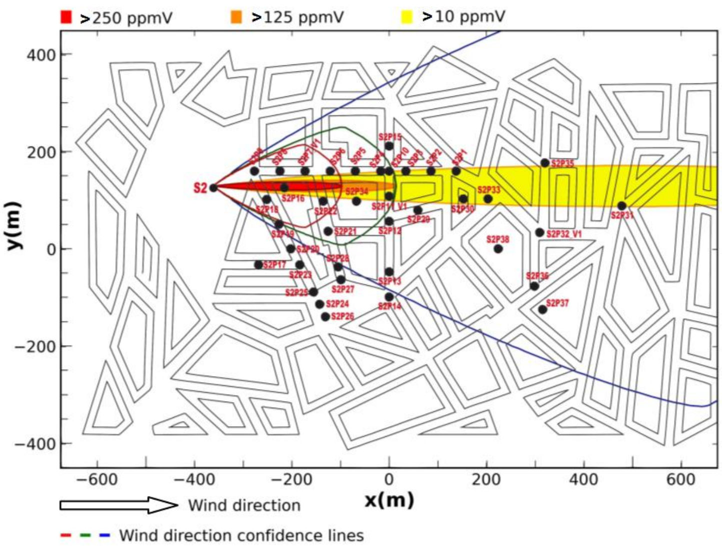

Figure 1. Horizontal distribution of average near ground concentrations for a continuous release from source S2 simulated with a models of type I (model 101).

A total of 21 different computational emergency response tools and were used in the COST ES1006 Michelstadt exercise. Given the varying airborne hazards flow and dispersion modelling approaches which are used in these models, the models can be grouped to the following tree model types according to their flow and dispersion modelling approach characteristics:

Type I – models that do not resolve the flow between buildings
Type II – models that the flow is resolved diagnostically or empirically, although not resolving the flow between buildings
Type III – models that resolve the flow between buildings

A summary of the models applied in the COST ES1006 Michelstadt exercise and the typical respective computational times needed for individual model runs in the exercise is given in table 2. The COST ES 1006 members decided to present all model results in common presentations anonymously. Therefore the models are addressed in terms of model numbers instead of model names in the following. The number of models used in the exercise and the number of groups of modellers involved are listed in table 3.

Table 2. Model approaches applied in the COST ES1006 Michelstadt exercise

Model type	Dispersion modelling method	Computational time
I	Gaussian (without / with building parameterization)	1 -5 minutes
II	Lagrangian dispersion models	2 minutes – 5 hours
III	CFD (RANS; LES; RANS-Lagrangian)	2 hours – 4 days

Table 3. Number of models and modellers participating in the Michelstadt test case release scenarios simulations considered in the COST ES1006 Michelstadt exercise

Model Type	Continuous Release		Puff Release	
	number of modellers	number of models	number of modellers	number of models
I	9	7	5	5
II	6	6	4	4
III	12	7	7	5

Most of the considered atmospheric dispersion models are ensemble average models. This type of models does not describe the behaviour of a single episode but the average of a large number of episodes. This approach could become critical when making simulations of experimental cases reproducing a strong variability among the outcomes of different realizations. Since the nature offers just one of these outcomes, the bias between simulations outcomes and reality could become critical for certain variables. This problem is less severe for the continuous emission experiments, where concentrations, being computed as time averages in stationary conditions, are substantially stable. In the puff cases, it is necessary to evaluate the significance of modelling results for certain indicators, showing a large experimental variability. This is particularly true for peak concentrations, whose meaningfulness has to be carefully verified also with the range or the distribution of experimental data. In case of a continuous release, maximum concentrations, dosages and especially the area affected by values above a relevant threshold usually are the information expected from an emergency response model.

Statistical comparisons in general test whether the simulated concentrations at receptor points (c_p) can match the observed concentration (c_0) and the degree of scatter. The primary quantitative performance measures are the fractional bias FB, the normalized mean square error NMSE and the fractions within a factor of two (FAC2). The following reference acceptance criteria are defined by Hanna and Chang (2012) for concentration simulations in built environment:
• |FB| < 0.67, i.e., the relative mean bias less than a factor of *2
• NMSE < 6, i.e., the random scatter < 2.4 times the mean
• FAC2 > 0.3, i.e., the fraction of Cp within a factor of two of Co that exceeds 0.3
It should be kept in mind that pairing concentration observations and predictions both in space and in time (for puffs) in statistical comparisons on these small scales is a very severe approach and the computed statistics may even describe worse results than actually obtained. Observed and simulated plumes may be very similar but small differences in the wind direction or in the representation of the buildings can make the plumes' overlap fail resulting in poor statistical paired indices. Observations which are instantaneous and single-point values may significantly differ from the time and space averages produced by a model. Finally, observed small-scale gradients between adjacent receptors are hardly captured by models due to spatial averaging.

RESULTS

Sensitivity to meteorological input parameters

The surface friction velocity u* of the approach flow calculated from the measured turbulent flow data and is 0.566 ms-1. However, over the Michelstadt domain, the surface roughness and therefore u* undergo some modifications. As a result, the approach flow vertical wind profile does not correspond to the conditions within the whole urban area. In order to quantify the impact of this effect on Gaussian model results not taking into account the flow between buildings (type I), sensitivity tests were made with u* varying between 62%u*0 [0.35 ms-1] and 100%u*0 [0.566 ms-1] and with z_0 between 0.5 m and 1.5 m. The statistical analysis revealed that in these cases, the best agreement between modelled concentrations at receptor points and measurements was found for u* = 71%u*0, z0 = 0.8 m (table 4).

Table 4. Selected results of the statistical comparison of model 107 concentrations for continuous release from source 2 to measurements for varying roughness lengths z_0 and friction velocities u_*

	u_* = 0.4 (71% u_{*0})		**u_* = 0.566 (100% u_{*0})**	
z_0	**FB**	**NMSE**	**FB**	**NMSE**
0.50	-0.06	1.01	0.47	1.75
0.80	0.01	0.88	0.57	1.56
1.00	0.05	0.85	0.61	1.52
1.25	0.11	0.84	0.67	1.51
1.50	0.14	0.85	0.70	1.53

As the models of type I do not simulate the variations of the flow field between the buildings, the choice of the input wind direction has a major effect on the location of the simulated plume. In practical applications, wind direction uncertainty is accounted for by depicting wind direction confidence lines in the maximum concentrations plot as shown in the upper picture of Figure 1. Sensitivity tests are undertaken in the Michelstadt exercise with two models of type I concerning variations in wind direction.

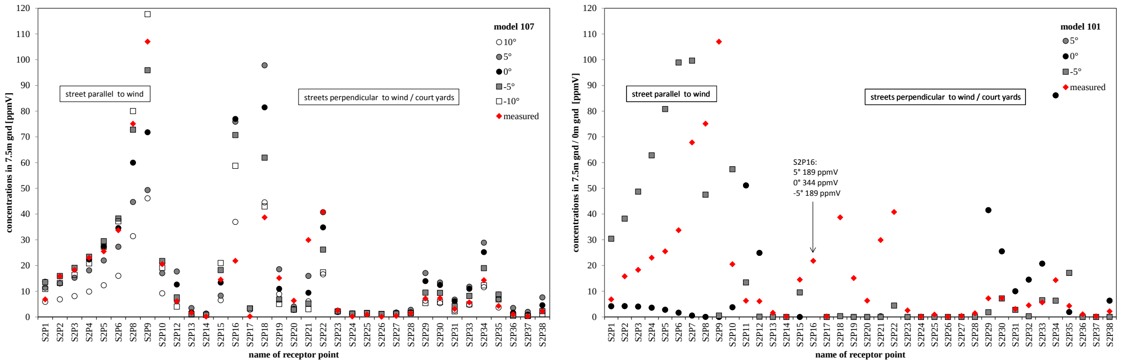

Figure 2. Comparison between measured and modelled average concentrations (left: model 107, right: model 101) for a continuous release from source S2 with variations in approach flow directions.

In figure 2, the average near ground concentrations (measurements and model 107 at 7,5m gnd; model 101 at 0m gnd) with varying inflow directions for a continuous release from source 2 are compared to the measured values. In the street parallel to the wind, where the receptors S2P1 to S2P10 are located, the measured concentrations are reproduced or overestimated when the inflow direction in the model is turned. Adding wind direction variations is not in all cases sufficient to catch all high concentration values when the flow field is affected by building structure influences: e.g. the concentrations at receptors S2P11 and S2P12 in a street perpendicular to the main flow are underestimated by all model results depicted in figure 2. Model 101 additionally underestimates the concentrations at S2P5 to S2P10. This is due to the fact that the plume width simulated with this model is comparably narrow (see figure 1).

Model performance according to model type

In Figure 3, all available model results of a model type that were calculated at the receptor points are averaged for each receptor point and compared to the respective measured value of the blind test cases. On the left side, simulated average concentration values within the street canyons (7.5m above ground) are compared to the measurements for all continuous release scenarios. On the right side, mean dosages simulated for puff releases are compared to the respective measurements. The bold line in the figures indicates optimal agreement. Within the dashed lines, model results and measurements agree within a factor of two. The agreement between the model ensemble values and the measurements increases with increasing complexity of the model approaches from model type I to type II and III. The model type I ensemble underestimates and overestimates the measured concentrations for more than a factor of two for the highest number of receptor locations. The type II ensemble renders less underestimation of more than a factor of two in the presented cases.

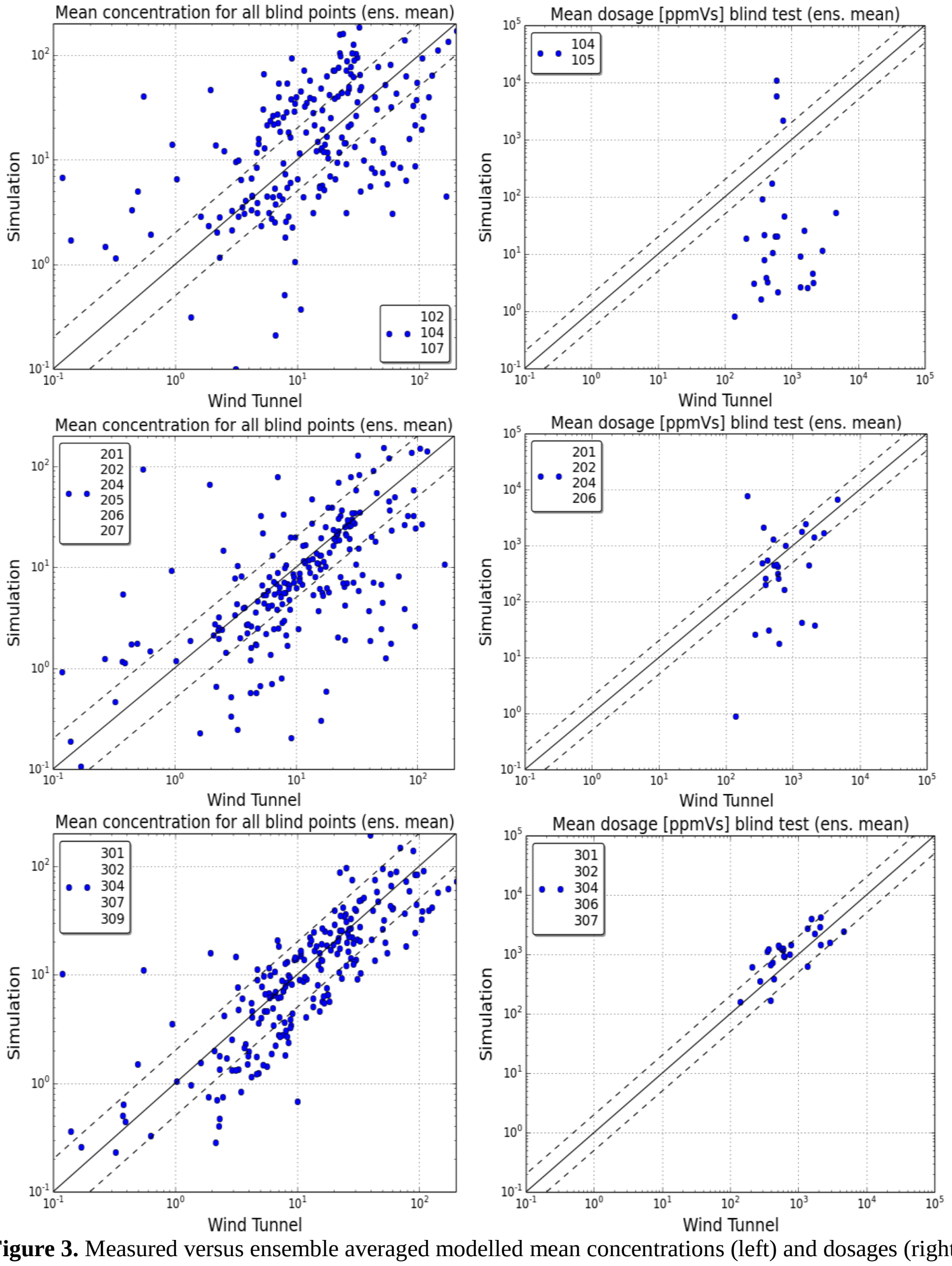

Figure 3. Measured versus ensemble averaged modelled mean concentrations (left) and dosages (right) at receptors for continuous releases (left) and puff releases (right) for model Type I (top left), II (top right) and III (bottom left).

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